Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Chiral Sensing of Amino Acids and Proteins Chelating with Eu^{III} Complexes by Raman Optical Activity Spectroscopy

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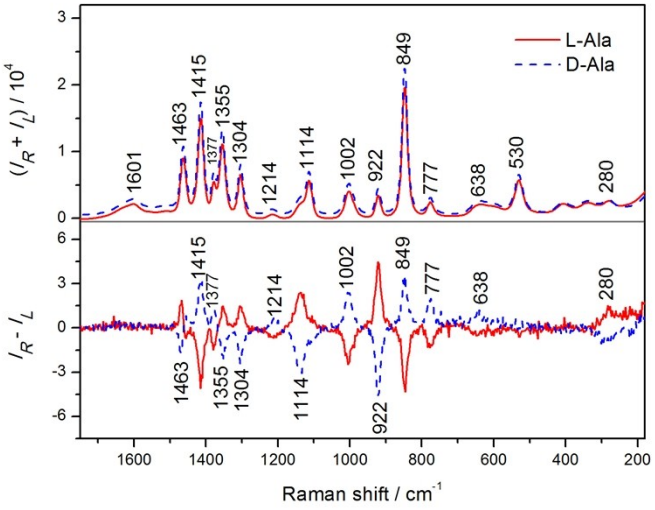

Figure S1. Raman (upper) and ROA (lower) spectra of L/D-alanine, 0.5 M aqueous solution.

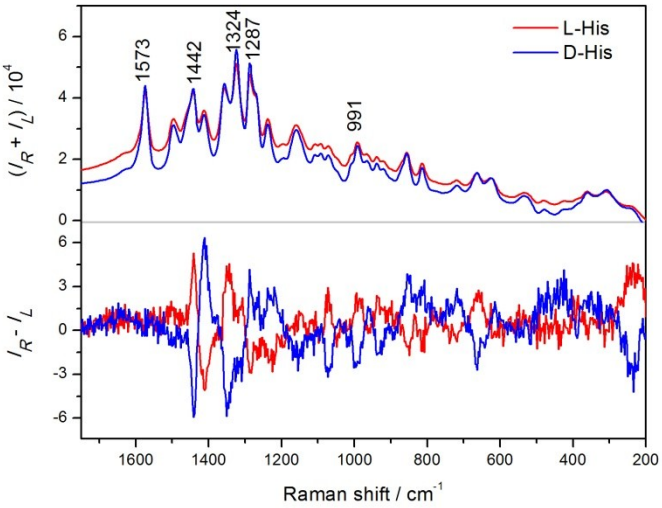

Figure S2. Raman (upper) and ROA (lower) spectra of L/D-histidine, 0.24 M aqueous solution.

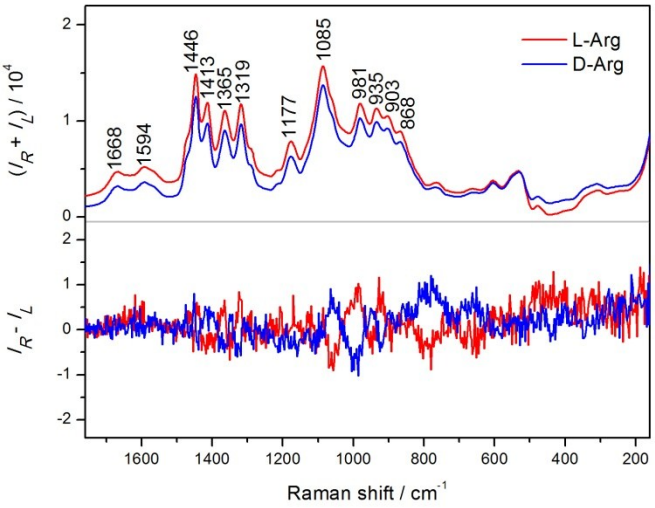

Figure S3. Raman (upper) and ROA (lower) spectra of L/D-arginine, 0.34 M aqueous solution.

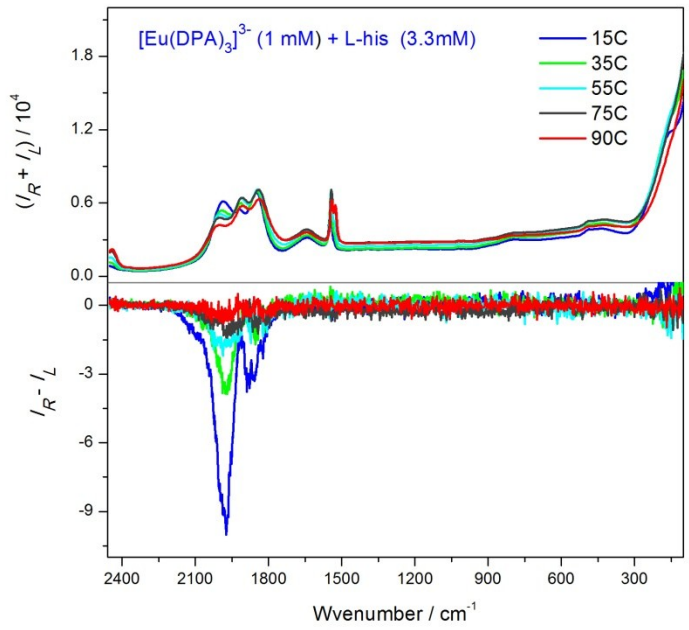

Figure S4. Raman (upper) and ROA (lower) spectra of the L-His-$[Eu(DPA)_3]^{3-}$ complex at different temperatures (pH = 2, accumulation times 20 minutes).

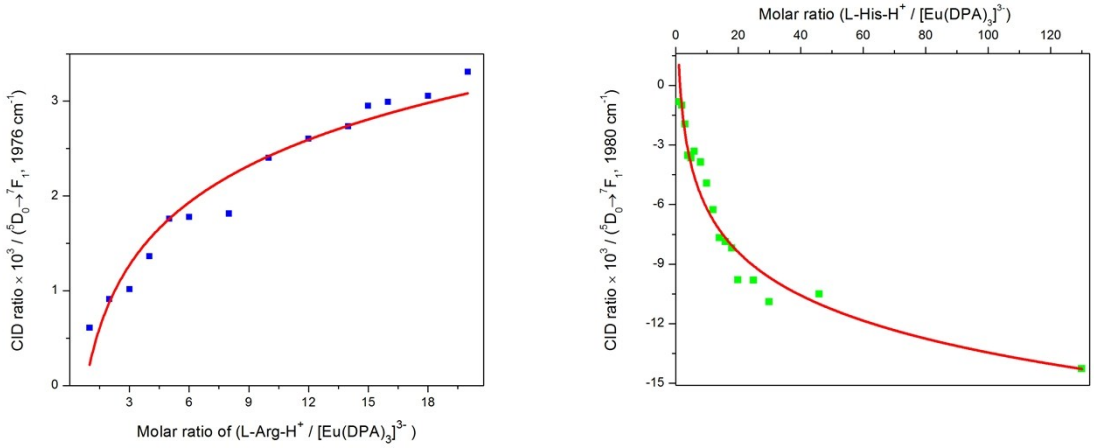

Figure S5. CID (ROA/Raman intensity ratio for the band at 1976 cm^{-1}) as dependent on the of L-Arg / $[Eu(DPA)_3]^{3-}$ molar ratio at pH = 7(left); and CID (ROA/Raman intensity ratio for the band at 1980 cm^{-1}) as dependent on the of L-His / $[Eu(DPA)_3]^{3-}$ molar ratio at pH = 2(right).

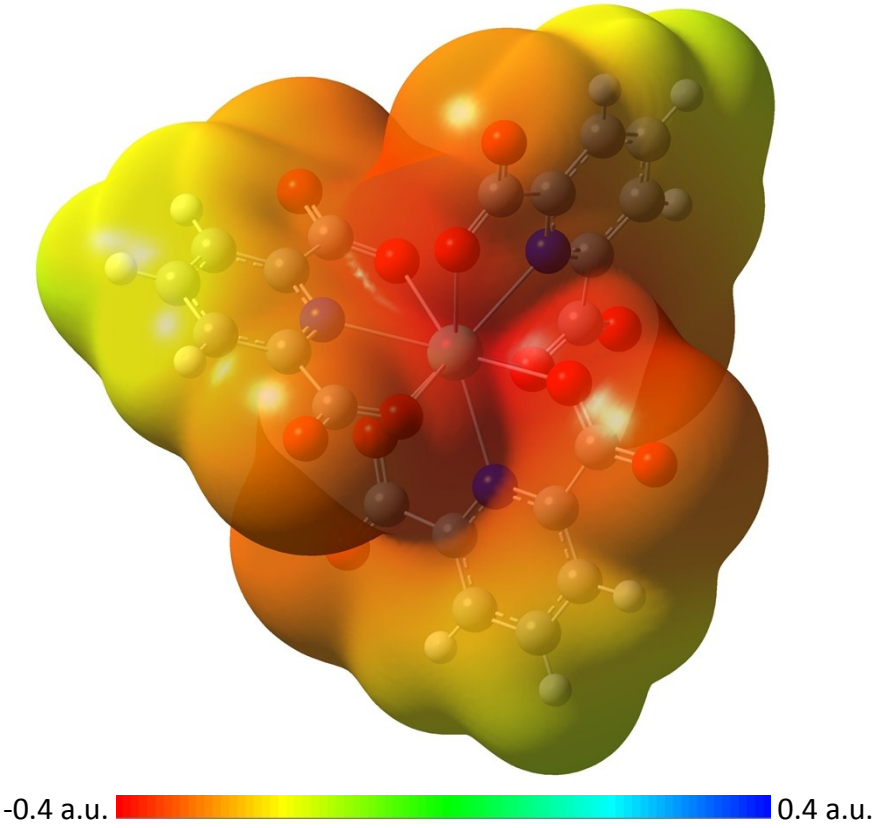

Figure S6. Calculated electrostatic potential of $[Eu(DPA)_3]^{3-}$.

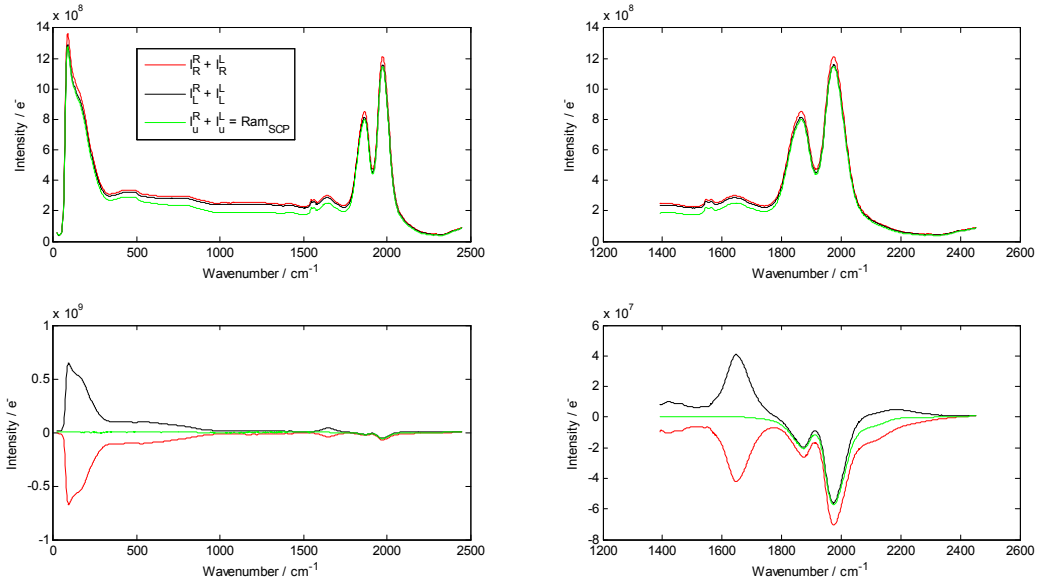

Figure S7. Raman (top) and degree of circularity (DOC, bottom) spectra of human lysozyme mixed with the $[Eu(DPA)_3]^{3-}$ complex, the polarization scheme is indicated in the inset. E.g., from the detail on the right hand side, one can recognize the true Raman scattering of water at 1650 cm^{-1} (opposite signs of the DOC bands) and circular polarized luminescence of Eu^{3+} at 1800-1100 cm^{-1} giving the same sign.

Table S1. CID ratios for selected $^5D_0 \rightarrow {}^7F_1$ transition of $[Eu(DPA)_3]^{3-}$ amino acids complexes

	Alanine		Arginine		Histidine	
Transition	ν / cm^{-1}	CID	ν / cm^{-1}	CID	ν / cm^{-1}	CID
$^5D_0 \rightarrow {}^7F_1$	1956	1.09×10^{-4}	2112	9.61×10^{-4}	1980	6.15×10^{-3}
pH 2	1866	7.87×10^{-5}	1970	6.19×10^{-4}	1872	2.51×10^{-3}
			1887	5.97×10^{-4}		
$^5D_0 \rightarrow {}^7F_1$	1976	4.78×10^{-5}	1976	1.76×10^{-3}	1976	1.94×10^{-4}
pH 7	1864	2.54×10^{-5}	1864	9.19×10^{-4}	1864	1.20×10^{-4}
$^5D_0 \rightarrow {}^7F_1$	1940	$\sim1\times10^{-5}$	1976	2.52×10^{-4}	1976	4.08×10^{-5}
pH 10	1860	$\sim1\times10^{-5}$	1864	7.31×10^{-5}	1864	3.54×10^{-5}